

THE HEAVILY DOPED SEMICONDUCTORS

By

R.Y. THAKUR

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PREFACE

The thesis is the result of untiring and unending guidance and assistance of Dr. D.K. Roy, Assistant Professor of Physics of I.I.T., Delhi whose aim in life, as I find, has been to unfold the mysteries of nature. Although trained to be an experimentalist, he has introduced the fundamental concept of energy distribution in field emission, needed to explain several long standing problems. Under his supervision the idea of the futility of impurity band concept is also being established and its impact on the physics of heavily doped semiconductors is being reported in this thesis.

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IIT Delhi

R.Y. Thakur
(R.Y. THAKUR)

ABSTRACT OF THE THESIS

The work to be described in the thesis has its genesis in our endeavour to grasp the physical basis of the formation of impurity bands in semiconductors doped with shallow state impurities. Analysed theoretically with great mathematical rigour and supported equally well by experimental measurements, currently these impurity bands form the heart of physics of heavily doped semiconductors. Apart from a number of seemingly convincing arguments in support of these bands, the partial ionisation of carriers in the heavy doping condition has often been used to support their existence. Recently it has been shown by Roy and George (1975), that the phenomenon of partial ionisation of carriers can also be explained without invoking the impurity band concept.

Applicability of perturbation theory at the band edge was questioned, as the bound states of impurities were regarded to exist in the heavy doping condition. But it was proposed by Mott (1949) and subsequently verified experimentally by Pearson and Bardeen (1949) and Debye and Conwell (1954), that shallow impurity states in semiconductors suddenly disappear around a doping concentration of about 10^{18} per cc. at room temperatures.

Prior to Mott transition, the impurity band formation due to overlap of bound electron wave functions is insignificant because the atoms are situated relatively at larger distances compared to impurity Bohr radius. Beyond this transition, the formation of such bands is again impossible since the bound state wavefunctions are non-existent, however strong may be the electron potential energy at a particular point. This effect may easily be conceived on the tight binding scheme of the energy band formation. Therefore, the possibility of formation of potential wells of arbitrary depths due to random distribution of impurity atoms, as has been argued by Kane and others can easily be ruled out; since the impurity ions have lost their strong attractive influences being highly screened by mobile electrons. At this stage the screened impurity centres may ideally be regarded to perturb the electron energy in the conduction band.

Binding energy calculations of impurities to shallow states are first undertaken in the thesis using the potentials of Thomas-Fermi and Hulthen to establish the futility of impurity band concept beyond impurity concentration of about 10^{18} per c.c. A density of states calculation in heavily doped semiconductors in the two band model using the coherent potential approximation is

thereafter carried out and compared with the perturbation calculation of Roy and George (1975). The latter was unable to account for the shift in the valence band edge of a strongly doped n-type semiconductor (say). Expressions for Fermi-energy level, Einstein relation and partial ionization of carriers as functions of doping and temperature are then derived and compared with experimental results. The thesis concludes with the calculation of temperature and pressure effects on band edges of heavily doped semiconductors. These have a direct bearing on the explanation of temperature and pressure dependences of peak current density in tunnel diodes. In the end, accounts of transport properties and dielectric functions of heavily doped semiconductors are added, and possible future lines of research are suggested.

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